Mixed and Implicit Schemes §3.2.4

The leapfrog scheme is stable for the oscillation equation and unstable for the friction equation.

The Euler forward scheme is stable for the friction equation but <u>unstable for the oscillation equation</u>.

Suppose we require an approximation to the equation

$$\frac{dU}{dt} = i\omega U - \kappa U \,,$$

This is a prototype of the N.S equations, with terms of both types.

One approach is to use the leapfrog scheme for the oscillation term and the forward scheme for the friction term:

$$U^{n+1} = U^{n-1} + 2\Delta t (i\omega U^n - \kappa U^{n-1}) \,. \label{eq:Unormalized}$$

We can show that this is stable provided

 $(2\kappa\Delta t+\omega^2\Delta t^2)\leq 1\,.$

The strongest constraint imposed by the CFL criterion is for the highest wave-speed c occurring in the system.

For the atmosphere, the speed of external gravity waves may be estimated as

$$c = \bar{u} + \sqrt{gH}$$

where \bar{u} is the advecting speed and H is the scale height.

We may assume $\bar{u} < 100 \,\mathrm{m \, s^{-1}}$ and $\sqrt{gH} < 300 \,\mathrm{m \, s^{-1}}$, so a safe maximum value for c is 400 m s⁻¹.

Then the maximum allowable time step for various spatial grid sizes may be estimated:

Δx :	200 km	$100 \mathrm{km}$	$20 \mathrm{km}$	$10 \mathrm{km}$
Δt :	$500 \mathrm{s}$	$250 \mathrm{\ s}$	$50 \mathrm{s}$	$25 \mathrm{s}$

In the two-dimensional case, the stability criterion is more stringent: we need to choose a time step that is $\sqrt{2}$ times smaller than that permitted in the one-dimensional case.

Modern numerical models of the atmosphere typically combine several distinct schemes in this way.

The Navier-Stokes equations are

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} + 2\mathbf{\Omega} \times \mathbf{V} + \frac{1}{\rho} \nabla p = \nu \nabla^2 \mathbf{V} + \mathbf{g}$$

They have advection terms corresponding to the oscillation equation and diffusion terms like the friction equation.

We will shortly consider the semi-implicit scheme, where some terms are integrated implicitly and others explicitly.

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NWP models also use various filtering processes to limit spatial and temporal noise.

Some of these represent diffusive physical processes. Others are just numerical damping, to prevent spurious noise.

Implicit Schemes

For the simple oscillation equation

$$\frac{dU}{dt} = i\omega U$$

the (centered) implicit approximation is

$$\frac{U^{n+1} - U^n}{\Delta t} = i\omega \left(\frac{U^{n+1} + U^n}{2}\right) \,.$$

This is second-order accurate and unconditionally stable:

$$U^{n+1} = \rho U^n$$
 where $\rho = \left(\frac{1 + \frac{1}{2}i\omega\Delta t}{1 - \frac{1}{2}i\omega\Delta t}\right)$

In this simple case, we may solve immediately for U^{n+1} . In general, we must solve a complicated nonlinear system.

Exercise: Verify that ρ is unimodular: $|\rho| = 1$.

The Semi-implicit Method (intro.)

It is common practice today to treat selected linear terms implicitly and the remaining terms explicitly.

The semi-implicit method was pioneered by André Robert.

The terms that give rise to high frequency gravity waves are integrated implicitly, enabling the use of a long time step.

Formally, we separate the terms into two groups.

Thus, the equation

$$\frac{du}{dt} = F(u) = F_1(u) + F_2(u)$$

is discretised by something like

$$\frac{U^{n+1} - U^{n-1}}{2\Delta t} = F_1(U^n) + F_2\left(\frac{U^{n-1} + U^{n+1}}{2}\right)$$

Schemes of this sort are pivotal in modern NWP models, due to their excellent stability properties.

Again, the CTCS or leapfrog scheme is

$$\left(\frac{U_m^{n+1} - U_m^{n-1}}{2\Delta t}\right) + c\left(\frac{U_{m+1}^n - U_{m-1}^n}{2\Delta x}\right) = 0$$

We now seek a solution of the form

$$U_m^n = U^0 \exp[ik(m\Delta x - Cn\Delta t)]$$

- If C is real, this is a wave-like solution.
- If C is complex, this solution will behave exponentially, quite unlike the solution of the continuous equation.

Substituting U_m^n into the FDE, we find that

$$C = \frac{1}{k\Delta t} \sin^{-1} \left[\left(\frac{c\Delta t}{\Delta x} \right) \sin k\Delta x \right]$$

Exercise: Verify this expression for C.

Distortion of the Phase Speed

We consider the simple 1-D advection equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \,,$$

where u(x,t) depends on both x and t.

The advection speed c is constant and, without loss of generality, we assume c > 0.

The equation has a general solution of the form u = f(x - ct), where f is an arbitrary function.

In particular, we may consider the sinusoidal solution $u = u(0) \exp[ik(x - ct)]$ of wavelength $L = 2\pi/k$.

We use centered difference approximations

$$\left(\frac{U_m^{n+1} - U_m^{n-1}}{2\Delta t}\right) + c\left(\frac{U_{m+1}^n - U_{m-1}^n}{2\Delta x}\right) = 0,$$

in both time and space (CTCS). Here $U_m^n = U(m\Delta x, n\Delta t)$.

Again,

$$C = \frac{1}{k\Delta t} \sin^{-1} \left[\left(\frac{c\Delta t}{\Delta x} \right) \sin k\Delta x \right] \,.$$

If the argument of the arcsine is less than unity, C is real. Otherwise, C is complex, and the solution grows with time. Clearly, $c\Delta t/\Delta x \leq 1$ is a sufficient condition for real C.

It is also necessary: for a wave of four gridlengths, we have $k\Delta x = \pi/2$, so that $\sin k\Delta x = 1$.

Thus, the condition for stability of the solution is

$$Le \equiv \frac{c\Delta t}{\Delta x} \le 1 \,.$$

This non-dimensional parameter is often called the Courant number, but is denoted here as Le for Lewy, who first discovered this stability criterion.

The above analysis may be repeated for an implicit discretization (six-point Crank-Nicholson scheme):

$$\frac{U_m^{n+1} - U_m^n}{\Delta t} + \frac{c}{2} \left(\frac{U_{m+1}^n - U_{m-1}^n}{2\Delta x} + \frac{U_{m+1}^{n+1} - U_{m-1}^{n+1}}{2\Delta x} \right) = 0.$$

Then the phase speed C of the numerical solution is

$$C = \frac{2}{k\Delta t} \tan^{-1} \left[\left(\frac{c\Delta t}{2\Delta x} \right) \sin k\Delta x \right] \,.$$

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Exercise: Verify this result. Hint: Substitute $U_m^n = U^0 \exp[ik(m\Delta x - Cn\Delta t)]$ into the equation.

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This equation contains an inverse tangent term instead of the inverse sine occurring in the leapfrog scheme.

Thus, the numerical phase speed C is always real, so the scheme is *unconditionally stable*.

Hints for MATLAB Exercise.

There are too many parameters. It is convenient to reduce the number by constructing non-dimensional quantities.

So, we define

$$\kappa = k \Delta x$$
 and $\mu = \frac{c \Delta t}{\Delta x}$.

Then the relationships can be written:

- $\frac{C}{c} = \frac{1}{\kappa\mu} \sin^{-1}(\mu \sin \kappa)$ for the explicit scheme.
- $\frac{C}{c} = \frac{1}{\kappa\mu} \tan^{-1}(\frac{1}{2}\mu\sin\kappa)$ for the implicit scheme.

Now there are only two parameters, κ and $\mu.$

You should plot curves of C/c as functions of μ for a selection of values of κ , say for $\kappa \in \{0, \frac{\pi}{10}, \frac{2\pi}{10}, \dots, \pi\}$, with μ varying from zero to, say, 10.

It is easily shown that $C \leq c$ and that $C \to \pi/k\Delta t$ as $c \to \infty$. Thus, the implicit scheme slows down the faster waves.

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MATLAB **Exercise**:

• Write a program to evaluate

$$C = \frac{1}{k\Delta t} \sin^{-1} \left[\left(\frac{c\Delta t}{\Delta x} \right) \sin k\Delta x \right] \,.$$

and determine the behaviour of C in the limits c = 0 and $c \longrightarrow \infty$.

• Write a program to evaluate

$$C = \frac{2}{k\Delta t} \tan^{-1} \left[\left(\frac{c\Delta t}{2\Delta x} \right) \sin k\Delta x \right] \,.$$

and determine the behaviour of C in the limits c = 0 and $c \longrightarrow \infty$.

Exercise.

Consider the four-point Crank-Nicholson scheme

$$\frac{1}{2} \left[\frac{U_m^{n+1} - U_m^n}{\Delta t} + \frac{U_{m+1}^{n+1} - U_{m+1}^n}{\Delta t} \right] + \frac{c}{2} \left[\frac{U_{m+1}^{n+1} - U_m^{n+1}}{\Delta x} + \frac{U_{m+1}^n - U_m^n}{\Delta x} \right] = 0$$

Show that the computational phase speed is given by

$$C = \frac{2}{k\Delta t} \tan^{-1} \left[\left(\frac{c\Delta t}{\Delta x} \right) \tan k\Delta x \right]$$

Hint.

Substitute $U_m^n = U^0 \exp[ik(m\Delta x - Cn\Delta t)]$ into the equation.

Implicit Time Schemes

In implicit schemes the advection or diffusion terms are written in terms of the new time level variables.

$$\mathbf{PDE:} \quad \frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$
$$\mathbf{FDE:} \quad \frac{1}{2} \left[\left(\frac{U_m^{n+1} - U_m^n}{\Delta t} \right) + \left(\frac{U_{m+1}^{n+1} - U_{m+1}^n}{\Delta t} \right) \right] \\ + c \left[\alpha \left(\frac{U_{m+1}^n - U_m^n}{\Delta x} \right) + (1 - \alpha) \left(\frac{U_{m+1}^{n+1} - U_m^{n+1}}{\Delta x} \right) \right] = 0$$

For $\alpha = \frac{1}{2}$, this is the four-point Crank-Nicholson scheme. The factor α determines the weight of the "old" time values compared with the "new" time values in the FDE. Using the von Neumann method, we substitute

$$U_m^n = A\rho^n e^{im\kappa} = Ae^{i(m\kappa - n\ell)}$$

into the FDE (where $\kappa = k \Delta x$ and $\theta = \omega \Delta t$).

Note that, for $\alpha = 1/2$, the scheme is centered in time at $U_{m+1/2}^{n+1/2}$ (which is not at a gridpoint in space or in time).

We multiply by $e^{-i\kappa/2}$ and obtain the amplification factor

$$\rho = \frac{\cos\frac{\kappa}{2} - i2\mu\alpha\sin\frac{\kappa}{2}}{\cos\frac{\kappa}{2} + i2\mu(1-\alpha)\sin\frac{\kappa}{2}} = \frac{1 - i2\mu\alpha\tan\frac{\kappa}{2}}{1 + i2\mu(1-\alpha)\tan\frac{\kappa}{2}}$$

Thus, the squared modulus of the amplification factor is

$$|\rho|^{2} = \frac{1 + 4\mu^{2}\alpha^{2}\tan^{2}\frac{\kappa}{2}}{1 + 4\mu^{2}(1 - \alpha)^{2}\tan^{2}\frac{\kappa}{2}}$$

This implies $\rho \le 1$ if $\alpha \le 0.5$, i.e., if the new values are given at least as much weight as the old values.

Again,

$$|\rho|^{2} = \frac{1 + 4\mu^{2}\alpha^{2}\tan^{2}\frac{\kappa}{2}}{1 + 4\mu^{2}(1 - \alpha)^{2}\tan^{2}\frac{\kappa}{2}}$$

For $\alpha \leq 0.5$, there is no restriction on the size of $\Delta t!$

Absolute stability — independent of the Courant number — is typical of implicit time schemes.

In an implicit scheme, a point at the new time level is influenced by all the values at the new level, which avoids extrapolation, and is absolutely stable.

Note also that if $\alpha < 0.5$ the implicit time scheme reduces the amplitude of the solution: it is an example of a damping scheme.

This property is useful for solving problems such as spuriously growing mountain waves in semi-Lagrangian schemes.



Schematic of an implicit scheme. Note that with the implicit scheme there is no extrapolation.

Summary I

If we consider a marching equation

$$\frac{dU}{dt} = F(U)$$

explicit methods such as the forward scheme

$$\frac{U^{n+1} - U^n}{\Delta t} = F(U^n)$$

or the leapfrog scheme

$$\frac{U^{n+1} - U^{n-1}}{2\Delta t} = F(U^n)$$

are either

- Conditionally stable, or
- Absolutely unstable.

Break here

Summary II

A fully implicit scheme

$$\frac{U^{n+1} - U^n}{\Delta t} = F(U^{n+1})$$

and a centered implicit scheme

$$\frac{U^{n+1}-U^n}{\Delta t}=F\left(\frac{U^n+U^{n+1}}{2}\right)$$

are absolutely stable.

The latter scheme is attractive because it is centered in time, and it can be written with centered space differences, which makes it second order in space and in time.

As these schemes have only two time levels, they have no computational mode.

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The Crank-Nicholson Scheme

The Crank-Nicholson Scheme is centered in both time and space.

It has good stability and accuracy properties. It is second order accurate and unconditionally stable.

Two forms of the Crank-Nicholson scheme for the advection scheme are commonly used:

• The four-point C-N scheme:

$$\frac{1}{2} \left[\frac{U_m^{n+1} - U_m^n}{\Delta t} + \frac{U_{m+1}^{n+1} - U_{m+1}^n}{\Delta t} \right] + \frac{c}{2} \left[\frac{U_{m+1}^{n+1} - U_m^{n+1}}{\Delta x} + \frac{U_{m+1}^n - U_m^n}{\Delta x} \right] = 0$$

• The six-point C-N scheme:

$$\frac{U_m^{n+1} - U_m^n}{\Delta t} + \frac{c}{2} \left[\frac{U_{m+1}^{n+1} - U_{m-1}^{n+1}}{2\Delta x} + \frac{U_{m+1}^n - U_{m-1}^n}{2\Delta x} \right] = 0$$

	Domain	of Deper	ndence (of Implic	it Schem	ıe
*	*	*	•	*	*	* n+1
1	1	•			1	
1	l I	•	l I		l I	
*	*•-	*	*	*	*	* n
1		l l		l I		l I
m-3	m-2	m-1	m	m+1	m+2	m+3

The line of bullets (•) represents a parcel trajectory.

The value at the point $m\Delta x$ at time $(n+1)\Delta t$ depends on all the points denoted by red asterisks (*).

Thus, the computational domain of dependence surrounds the physical domain of dependence.

This is a necessary condition for a stable scheme.

Example of a Linear System.

The 1-D advection equation on a periodic domain is

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$
 $u(L,t) = u(0,t)$

The implicit scheme (six-point Crank-Nicholson) scheme is

$$\frac{U_m^{n+1} - U_m^n}{\Delta t} + \frac{c}{2} \left[\frac{U_{m+1}^{n+1} - U_{m-1}^{n+1}}{2\Delta x} + \frac{U_{m+1}^n - U_{m-1}^n}{2\Delta x} \right] = 0$$

We can write this in matrix form (with $\mu = c\Delta t/4\Delta x$)

$$\begin{bmatrix} 1 & +\mu & 0 & \dots & -\mu \\ -\mu & 1 & +\mu & \dots & 0 \\ 0 & -\mu & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ +\mu & 0 & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} U_0^{n+1} \\ U_1^{n+1} \\ \vdots \\ U_{M-1}^{n+1} \end{bmatrix} = \begin{bmatrix} 1 & -\mu & 0 & \dots & +\mu \\ +\mu & 1 & -\mu & \dots & 0 \\ 0 & +\mu & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mu & 0 & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} U_0^n \\ U_1^n \\ U_2^n \\ \vdots \\ U_{M-1}^n \end{bmatrix}$$

where $x_M = M \Delta x$ and $U_M^n = U_0^n$ for all n.

Implicit Schemes & Linear Systems

All implicit schemes also have a significant disadvantage.

Since U^{n+1} appears on the left- and on the right-hand sides, the solution for U^{n+1} , requires the solution of a system of equations.

If it involves only tridiagonal systems, this is not an obstacle, because there are fast methods to solve them.

There are also methods, such as fractional steps (with each spatial direction solved successively), where one space dimension is considered at a time.

These so-called ADI (alternating direction implicit) schemes allow large time steps without a large additional computational cost.

Symbolically, the equation may be written

$$\mathbf{M}_1 \mathbf{U}^{n+1} = \mathbf{M}_2 \mathbf{U}^n$$

The formal solution of this is

$$\mathbf{U}^{n+1} = \mathbf{M}_1^{-1}\mathbf{M}_2\mathbf{U}^n$$

However, this requires the inversion of an $M \times M$ matrix. There are much better ways to solve it.

The matrix M_1 is periodic tri-diagonal. There are very efficient numerical methods of inverting a system with such a matrix.

The non-periodic problem, with U_0^n and U_M^n given, results in a slightly different matrix, also tri-diagonal.

If the non-linear terms are treated implicitly, we must solve a nonlinear algebraic system every time step.

This is normally *impractical*.

The possibility of using a time step with a Courant number much larger than 1 in an implicit scheme does not guarantee that we will obtain accurate results economically.	
The implicit scheme maintains stability by slowing down the solutions, so that the waves satisfy the CFL condition.	
We saw this clearly in the analysis of the six-point Crank- Nicholson scheme.	
For this reason, implicit schemes are useful for those modes that are very fast but of little meteorological importance.	Conclu
We will next consider schemes in which the gravity wave terms are implicit while the remaining terms are explicit.	
These semi-implicit schemes are of crucial importance in modern NWP.	
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Exercise: See Notes and Exercises, Kalnay, pp. 87–88.	
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